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Report Title

ESTABLISHMENT OF A CENTER FOR DEVELOPMENT OF CHEMICAL SENSORS FOR EXPLOSIVES AT UNIVERSITY OF PUERTO RICO–MAYAGÜEZ

ABSTRACT

DoD-UPRM-MURI grant: “Establishment of a Center for Development of Chemical Sensors for Explosives at University of Puerto Rico – Mayaguez” (Proposal # 43567CHMUR; Agreement #: DAAD190210257) operated between 2002 and 2010. The project established a multidisciplinary research center for detection of landmine explosives, focusing on spectroscopic signatures of landmines explosives and transport in soil, contributing to real time chemical sensing of landmines. Goals included:

- * Measurement of spectroscopic signatures of landmine explosives in soil;
- * Measurement of effect of environmental variables on explosives;
- * Studies of soil-explosives interactions: Raman and IR spectroscopies
- * Model transport behavior of explosives in soils under different environmental conditions.

During the last 8 years of operation, the Center for Chemical Sensors Development (CCSD) studied the detection of high explosives and homemade explosives from near field under a microscope to far field at standoff distances. Research included synthesis and characterization of explosives: nitroaliphatic and cyclic organic peroxides. Studies also included transport of explosives in soils, both physical and mathematical modeling. The DoD sponsored research center has served to train and educate a significant number of students from BS to Ph.D. levels.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1. Espinosa-Fuentes, E.A., Peña-Quevedo, A.J., Pacheco-Londoño, L.C., Infante-Castillo, R. and Hernández-Rivera, S.P., A Review of Peroxide Based Homemade Explosives: Characterization and Detection, in "Explosive Materials: Classification, Composition and Properties", Janssen, T.J., ed., Chemical Engineering Methods and Technology Series, Nova Science Publishers, Inc. Hauppauge, NY, fourth quarter 2010, ISBN: 978-1-61761-188-9.
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Number of Papers published in peer-reviewed journals: 35.00

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160. Tatiana Luna-Pineda, Kristina Soto-Feliciano, Edwin De La Cruz-Montoya, Carlos Ríos-Velázquez and Samuel P. Hernández-Rivera, Spectroscopic Characterization of Biological Agents Using Normal Raman and Surface Enhanced Raman Spectroscopy, MURI-UPRM Program Annual Review Meeting, Mayagüez Resort and Casino, Mayagüez, PR, March 6-7, 2007.
161. William Ortiz, Doris Nunez-Quintero, Leonardo C. Pacheco-Londoño and Samuel Hernández-Rivera, Spectroscopic Modeling of Nitro Group in Explosives, MURI-UPRM Program Annual Review Meeting, Mayagüez Resort and Casino, Mayagüez, PR, March 6-7, 2007.
162. Yadira Soto-Feliciano, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera, Temperature Dependence of Detection Limits of TNT on Metallic Surfaces using Fiber Optic Coupled FTIR, MURI-UPRM Program Annual Review Meeting, Mayagüez Resort and Casino, Mayagüez, PR, March 6-7, 2007.
163. Deborah Nieves, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera. Chemical Warfare Agents Stimulants (CWAS) Detection on different surfaces using Fiber Optic Coupled Grazing Angle Probe-FTIR, Puerto Rico Interdisciplinary Scientific Meeting (PRISM 2007) and Junior Technical Meeting 2007, Interamerican University of Puerto Rico, Bayamón Campus, PR, March 10, 2007.
164. Nelmarie Rodriuez, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera 2, 4, 6-trinitrotoluene on Non Traditional Surfaces: Fiber Optic Coupled Grazing Angle Probe- FTIR Detection, Puerto Rico Interdisciplinary Scientific Meeting (PRISM 2007) and Junior Technical Meeting 2007, Interamerican University of Puerto Rico, Bayamón Campus, PR, March 10, 2007.
165. Oliva M. Primera-Pedrozo, Yadira M. Soto-Feliciano, Evamari Figueroa-Mass, and Leonardo C. Pacheco-Londoño and Samuel P. Hernández-Rivera. Gold Nanorods at Different Aspect Ratios for Surface-Enhanced Raman Scattering (SERS) Applications. Puerto Rico Interdisciplinary Scientific Meeting (PRISM 2007) and Junior Technical Meeting 2007, Interamerican University of Puerto Rico, Bayamón

Campus, PR, March 10, 2007.

166. Kristina Soto, Tatiana Luna and Samuel P. Hernandez-Rivera, Spectroscopic Characterization of Biological Agents Using Normal Raman and Surface Enhanced Raman Scattering. Puerto Rico Interdisciplinary Scientific Meeting (PRISM 2007) and Junior Technical Meeting 2007, Interamerican University of Puerto Rico, Bayamón Campus, PR, March 10, 2007.
167. Alvaro J. Peña-Quevedo, Robert B. Cody, Nairmen Mina-Calmide, and Samuel P. Hernández-Rivera, Synthesis, Characterization and Identification of Tetramethylene Diperoxide Dicarbamide by Direct Analysis Real Time –Mass Spectrometry and Vibrational Microscopy, 233rd American Chemical Society Meeting, Chicago, IL, March 25-29, 2007.
168. Kristina Soto-Feliciano, Tatiana Luna-Pineda, Edwin De La Cruz-Montoya, Carlos Ríos-Velázquez and Samuel P. Hernández-Rivera, “Spectroscopic Characterization of Biological Agents Using Normal Raman and Surface Enhanced Raman Spectroscopies”, 3rd Latin American and Caribbean Biotechnology Congress, Mayagüez, PR, September 22, 2006.
169. Bibiana Báez, Vivian Florián, Samuel P. Hernández-Rivera*, Andrea Cabanzo, Sandra Correa, Maik Irrazábal, Julio G. Briano, Miguel E. Castro, “Detection of chemical signatures from TNT buried in sand at various ambient conditions” American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
170. Deborah Nieves, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera, “Detection of Chemical Warfare Agents Simulants (CWAS) using Fiber Optic Coupled Grazing Angle Probe-FTIR”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
171. Alvaro J. Peña-Quevedo, Robert B. Cody, Nelmarie Rodríguez, Deborah Nieves, Miguel Castro-Rosario, Nairmen Mina-Camide, and Samuel P. Hernández-Rivera, “Synthesis, Characterization and Differentiation of High Energy Amine Peroxides by DART-TOF-MS and Vibrational Microscopy”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
172. Gabriel Perez, Edwin De La Cruz, Victor De La Cruz, Leonardo C. Pacheco and Samuel P. Hernández-Rivera, “Structural properties and Photodegradation Kinetic relationships of explosives with TiO₂ nanoparticles”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
173. Gloria Marcela Herrera-Sandoval, Luz Marina Ballesteros, Nairmen Mina, Julio Briano, and Samuel P. Hernández-Rivera, “Vibrational Signatures of TNT-Montmorillonite Clay Particles”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
174. Maik Irrazábal, Vivian Florián, Samuel P. Hernández-Rivera, and Julio G. Briano, “Fate and Transport of ERCs in Soil from Landmine Emissions, Numerical Simulations”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
175. Jackeline I. Jeréz-Rozo, Ana Maria Chamoun, Joany Hernández and Samuel P. Hernández-Rivera, “Enhanced Raman scattering of nitro-explosives on nanoparticle substrates: Ag and Au colloids and Au-Ag alloy”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
176. Leonardo Pacheco-Londoño, Oliva M. Primera-Pedrozo and Samuel P. Hernández-Rivera, “Standoff Infrared Detection of Explosives at Laboratory Scale”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
177. Nelmarie Rodríguez –Cardona, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera, “Detection of 2, 4, 6-Trinitrotoluene on Surfaces using Fiber Optic Coupled Grazing Angle Probe- FTIR, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
178. Ricardo Infante-Castillo and Samuel P. Hernández-Rivera, “Theoretical and experimental vibrational and NMR studies of RDX”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
179. Sandra Peña Edwin de la Cruz, Samuel P. Hernández-Rivera, “Development of SPME – HPLC Methodology for Detection of Nitroexplosives”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
180. Tatiana Luna-Pineda, Kristina Soto-Feliciano, Edwin De La Cruz-Montoya, Carlos Ríos-Velázquez and Samuel P. Hernández-Rivera, “Spectroscopic Characterization of Biological Agents Using Normal Raman and Surface Enhanced Raman Spectroscopy”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
181. Yadira Soto-Feliciano, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera, “Temperature Dependence of the Limits of Detection of TNT on Metallic Surfaces using Fiber Optic Coupled-FTIR”, American Chemical Society, Puerto Rico Section, 30th Senior Technical Meeting, November 3-4, 2006.
182. Alvaro J. Peña-Quevedo, Robert B. Cody, Nelmarie Rodríguez, Deborah Nieves, Miguel Castro-Rosario, Nairmen Mina-Camide and Samuel P. Hernández-Rivera, “Characterization and Differentiation of High Energy Amine Peroxides by DART-TOF-MS and Vibrational Microscopy”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
183. Bibiana Báez, Vivian Florián, Samuel P. Hernández-Rivera, Andrea Cabanzo, Sandra Correa, Maik Irrazabal, Julio G. Briano, Miguel E. Castro, Detection of chemical signatures from TNT buried in sand at various ambient conditions”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
184. Deborah Nieves, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera, “Detection of Chemical Warfare Agents Simulants (CWAS) using Fiber Optic Coupled Grazing Angle Probe-FTIR”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
185. Gabriel Perez, Edwin De La Cruz, Victor De La Cruz, Leonardo C. Pacheco and Samuel P. Hernández-Rivera, “Photodegradation

- Kinetics of explosives with TiO₂ nanoparticles”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
186. Gloria Marcela Herrera-Sandoval, Luz Marina Ballesteros, Nairmen Mina, Julio Briano and Samuel P. Hernández-Rivera, “FTIR and Raman Signatures of TNT –Montmorillonite Clay Particles”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
187. Jackeline I. Jeréz-Rozo, Ana Maria Chamoun, Joany Hernández and Samuel P. Hernández-Rivera, “Detection of nitro-explosives by Enhanced Raman scattering on nanoparticle substrates: Ag and Au colloids and Au-Ag alloy”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
188. Leonardo Pacheco-Londoño, Oliva M. Primera-Pedrozo and Samuel P. Hernández-Rivera, “Detection of Explosives by Standoff Infrared at Laboratory Scale”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
189. Nelmarie Rodríguez –Cardona, Oliva M. Primera-Pedrozo, Leonardo Pacheco-Londoño and Samuel P. Hernandez-Rivera, “Fiber Optic Coupled Grazing Angle Probe- FTIR Detection of 2, 4, 6-Trinitrotoluene on Surfaces”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
190. Ricardo Infante-Castillo and Samuel P. Hernández-Rivera, Theoretical and experimental vibrational and NMR studies of RDX, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
191. Sandra Peña, Edwin de la Cruz, Samuel P. Hernández-Rivera, “Development of SPME – HPLC Methodology for Detection of Nitroexplosives”, EXPOCHEM 2006, University of Puerto Rico Mayagüez, Mayagüez, PR, November 91-11, 2006.
192. Tatiana Luna-Pineda, Kristina Soto-Feliciano, Edwin De La Cruz-Montoya, Carlos Ríos-Velázquez and Samuel P. Hernández-Rivera, “Normal Raman and Surface Enhanced Raman Spectroscopy Detection of Biological Agents”, EXPOCHEM 2006, University of Puerto Rico, Mayagüez, PR, November 9-11, 2006.
193. Vibrational Spectroscopy of Explosives: From the Research Lab to Field Experiments, Samuel P. Hernández-Rivera, 9th Annual Army Landmine Basic Research Technical Review Meeting, Sponsored by the Army Research Office and the Joint Unexploded Ordnance Coordination Office, Springfield, Virginia, February 2006.
194. Samuel P. Hernández-Rivera, MURI Center For Chemical Sensors Development: Program Overview, Real-Time Explosive Specific Chemical Sensors MURI Review Big Sky, Montana, February 2006.
195. Samuel P. Hernández-Rivera, Vibrational Spectroscopy of Explosives, Real-Time Explosive Specific Chemical Sensors MURI Review Big Sky, Montana, February 2006.
196. Julio Briano, Review of Numerical Simulation of Fate and Transport of ERCs in Soil from Landmine Emissions, Real-Time Explosive Specific Chemical Sensors MURI Review Big Sky, Montana, February 2006.
197. Julio Briano, Finite Volume Elements Calculation of Transport of Explosives in Soils, Real-Time Explosive Specific Chemical Sensors MURI Review Big Sky, Montana, February 2006.
198. Julio Briano, Fate and Transport of TNT from Landmines, a Numerical Approach, 9th Annual Army Landmine Basic Research Technical Review Meeting, Sponsored by the Army Research Office and the Joint Unexploded Ordnance Coordination Office, Springfield, Virginia, February 2006.
199. Yadira Soto-Feliciano, Fiber Optic Coupled – Reflection Absorption Infrared Spectroscopy: Development of Sensitive and Robust Quantitative Analysis Methodology of Traces of Organic Residues on Surfaces, Proceedings of The National Conference on Undergraduate Research (NCUR) 2006, The University of North Carolina at Asheville, Asheville, North Carolina, April 6 – 8, 2006.
200. Alia El Burai-Félix, SER(R)S of Gold and Silver Metal Colloidal Film Deposited on a Flexible Polymer Substrate, 26th Puerto Rico Interdisciplinary Scientific Meeting, 41st Junior Technical Meeting, Cayey, PR, March, 2006.
201. Yadira Soto-Feliciano, TNT and PETN on surfaces: Grazing Angle – FTIR, 26th Puerto Rico Interdisciplinary Scientific Meeting, 41st Junior Technical Meeting, Cayey, PR, March, 2006.
202. Samuel P. Hernández-Rivera, Vibrational Spectroscopy of Chemical Agents and Toxic Vapors: From the Research Lab to Field Experiments, 2006 International Symposium on Spectral Science Research, Bar Harbor ME, June, 2006.
203. Samuel P. Hernández-Rivera, Center For Chemical Sensors Development, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.
204. Samuel P. Hernández-Rivera, Vibrational Spectroscopy Applied to IED Defeat: From The Research Lab to Field Experiments, UXO/Countermine/Range, Forum 2006, Las Vegas, Nevada, July, 2006.
205. Rosángela Rivera, Liliana Alzate, Neisa M. Hernandez, Samuel P. Hernandez, and Nairmen Mina, Adsorption of TNT on clay minerals, 231st ACS National Meeting & Exposition, Atlanta GA, March 26-30, 2006.
206. Neisa M. Hernandez, Rosángela Rivera, Liliana Alzate, Yleana Colon, Samuel P. Hernandez, and Nairmen Mina Molecular orbital calculations of the RDX-siloxane surface complex, 231st ACS National Meeting & Exposition, Atlanta GA, March 26-30, 2006.
207. Leonardo C. Pacheco, Vibrational spectroscopy study of triacetone triperoxide: Experimental and DFT Theoretical Studies, XXXI Congreso de Químicos Teóricos de Expresión Latina (“Congress of Theoretical Chemist of Latin Expression”), QUITEL2005, Margarita Island, Venezuela, October 2-6, 2005.
208. Oliva M Primera, Stability and Verification of TATP Fragment Cations in Gas Phase: Mass Spectrometry and DFT Theoretical Studies, XXXI Congreso de Químicos Teóricos de Expresión Latina (“Congress of Theoretical Chemist of Latin Expression”), QUITEL2005,

Margarita Island, Venezuela, October 2-6, 2005.

209. Yadira Soto, TNT and PETN on surfaces: Grazing Angle – FTIR, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005

210. Álvaro J. Peña, Analytical Methodology for Identification and Trace Analysis of Cyclic Acetone Peroxide Compounds by GC-MS, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

211. Neisa M. Hernández, Liliana Alzate, Rosangela Rivera, Samuel P. Hernández and Nairmen Mina. Interactions and vibrational spectroscopic signature of TNT in soil. XXIX ACS Senior Technical Meeting, Lajas P.R., November 2005.

212. Padilla, Ingrid, Diego Perez, and Juan Pablo Gutierrez, Two-Dimensional Modeling Of The Fate And Transport Of Explosive Chemicals Near Soil-Atmospheric Interfaces Subjected to Advection Processes, Poster presentation in Geological Society of America Annual Conference, Salt Lake City, Utah, October 16-19, 2005.

213. Perez, Diego, David Hernandez, and I. Padilla, Physical Modeling of the Fate and Transport of Explosive Chemicals in 1-D Soil Columns Subjected to Advection Processes, Poster Presentation in 25th Puerto Rico Interdisciplinary Scientific Meeting and 40th ACS Junior Technical Meeting, March 12, 2005.

214. Torres, Alexander and I. Padilla, Physical Modeling of Explosive Chemicals Diffusion in Soils Under Variable Environmental Conditions, Poster Presentation in 25th Puerto Rico Interdisciplinary Scientific Meeting and 40th ACS Junior Technical Meeting, March 12, 2005.

215. Tarafa, P. A. Torres, V. Vargas, and I. Padilla, Transport of Landmine-Derived Chemicals in Different Soils Under Variable Environmental Conditions, Poster Presentation in 25th Puerto Rico Interdisciplinary Scientific Meeting and 40th ACS Junior Technical Meeting, March 12, 2005.

216. Carmen M. Ramos, Neisa M. Hernandez, Rosángela Rivera, Liliana Alzate, Yleana Colon, Samuel P. Hernandez, and Nairmen Mina Density Functional Theory Treatment of the Structures and Vibrational Frequencies of 2,4- and 2,6-dinitrotoluenes. XXXI Congreso de Químicos Teóricos de Expresión Latina (QUITEL2005) Venezuela, Octubre 2-6, 2005.

217. Michael L. Ramírez, Characterization of Energetic Compounds Using Differential Scanning Calorimetry, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

218. Oliva M. Primera, TNT and PETN on surfaces: Grazing Angle – FTIR, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

219. Álvaro J. Peña, Method Development for Trace Detection and Differentiation of High Energy Cyclic Peroxide by Vibrational Microscopy, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

220. Bibiana Báez, Detection of Explosives in Soils using SPME with Gas Chromatography and TEEM –Mass Spectrometry, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

221. Edwin de la Cruz, Surface Enhanced Raman Spectroscopy of 2,4,6-Trinitrotoluene in Anatase Nanocrystal, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

222. Indira Jerez-Rozo, Raman Scattering of Nitroexplosives on Nanoscaled Substrates: Tungsten Trioxide, Copper (I) Oxide, Molybdenum (VI) Oxide, Tin (IV) Oxide, Cobalt (II, III) Oxide, Cerium (IV) Oxide And Scandium Oxide, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

223. Leonardo C. Pacheco, Nitroexplosives Classification by Molecular Descriptors, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

224. Luz M. Ballesteros, Raman Spectroscopic Signatures of PETN in Soil, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

225. Gloria M. Herrera, Vibrational Raman Signatures of TNT in Contact with Sand Particles, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

226. Marcia del R. Balaguera, SERS(S) of Metal Colloidal Polymeric Film, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

227. Michael L. Ramírez, Thermal Ink Jet Based Sample Transfer Techniques for Explosives Detection, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.

228. Hernandez-Rivera, S.P., “Spectroscopic Signature of Landmine Components in Soil and its Equilibrium Vapor: The First Step Towards Real-Time Landmine Sensing”, 7th Annual Army Landmine Basic Research Technical Review Meeting, Alexandria, VA, February 24-25, 2004.

229. Hernández-Rivera, S.P., “Detection of Explosives via Spectroscopic Signatures”, Workshop for Improvised Explosive Device (IED) Locating Through Explosives Detection, Night Vision and Electronic Sensors Directorate, Institute for Defense Analysis, Alexandria, VA, July 1, 2004.

Number of Presentations: 229.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

0

(d) Manuscripts

Number of Manuscripts:

0.00

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Leonardo C. Pacheco-Londoño	1.00
Oliva M. Primera-Pedrozo	1.00
Gloria M. Herrera-Sandoval	1.00
Bibiana Baez-Angarita	1.00
Sandra N. Correa-Torres	1.00
Luz M. Ballesteros	1.00
Alvaro Peña-Quevedo	1.00
Michael L. Ramirez-Cedeño	1.00
Ricardo Infante-Castillo	0.10
Lewis Gomez	1.00
Andrea Cabanzo	1.00
Tatiana Luna	1.00
Edwin de la Cruz	1.00
Victor de la Cruz	1.00
Marcia Balaguera	1.00
William Ortiz	1.00
Orlando Ruiz-Pesante	0.10
Marcos Barreto	0.10
Alejandro Blanco	1.00
Nelson Granda	0.20
Pedro Fierro	0.50
Yleana Colon	1.00
Indira Jerez	1.00
Maik Irrazabal	1.00
Celia Osorio	1.00
Liliana Alzate	1.00
Carmen Ramos	1.00
Neiza Hernandez	1.00
Carlos Peroza	1.00
Miguel Gonzalez	1.00
Hisamar Felix	1.00
Omar Rivera-Betancourt	1.00
José Luis Ruiz	1.00
Eduardo Espinosa	1.00
John Castro	1.00
Dustin Perez	1.00
Vivian Florian	1.00
Miguel Florian	1.00
Ernesto Borrero	
Enid Colon	1.00
Cynthia Caraballo	1.00
Jose Rivera	1.00
Rafael Rivera	1.00
Jose A. Santiago	1.00
Ivonne Feliciano	1.00
Sandra Peña	1.00
Angel Anaya	1.00
Jose Falcon	1.00
Gloria Molina	1.00
Alexander Torres	1.00
Cesar Manrique	
Rosangela Rivera	1.00
FTE Equivalent:	46.00
Total Number:	52

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Alberto Santana	1.00
Jairo Castollo-Chara	1.00
FTE Equivalent:	2.00
Total Number:	2

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Samuel P. Hernandez-Rivera	0.35	No
Ingrid Padilla	0.25	No
Julio Briano	0.25	No
Nairmen Mina-Camilde	0.25	No
Miguel Castro-Rosario	0.25	No
Sangchul Hwang	0.25	No
FTE Equivalent:	1.60	
Total Number:	6	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Migdalia Hidalgo Santiago	
Sujeily Soto Medina	
Nancy Soto Acevedo	
Juan Santa Roman	
Jeylisse Castaner De Choudens	
Rosa I. Martinez Garcia	
Rhaisa Sanchez Cuprill	
Francesca Rios Miller	
Gabriela D.Rodriguez Gonzalez	
Darlyn Mercado Saldivia	
Katia Y.Lasanta Pagán	
Jean Melendez Degro	
Gabriel A.Nieves Colon	
Lorena Marrero Vilches	
Jaleidy Hernandez	
Roxannie Gonzalez	
Cristie Cordero Velazquez	
Christine Jusino Olivencia	
Marilyn M. Cancel	
Alice Arroyo Oquendo	
Cristina Alicea Matos	
FTE Equivalent:	
Total Number:	21

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	61.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	58.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	45.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):	27.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	5.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	5.00

Names of Personnel receiving masters degrees

NAME

Oliva M. Primera-Pedrozo
Leonardo Pacheco-Londoño
Alejandro Blanco
Bibiana Baez-Angarita
Sandra N. Correa-Torres
Lewis Gomez
Sandra Peña
Indira Jerez
Tatiana Luna
Luz M Ballesteros
Gloria M. Herrera
Edwin de la Cruz
Liliana Alzate
Yleana Colon
Ernesto Borrero
Jose Luis Ruiz
Eduardo Espinosa
John Castro
Marcia Balaguera
Andrea Cabanzo
Omar Rivera-Betancourt
Pedro Fierro
William Ortiz
Alexander Torres
Angel Anaya
Luis Rivera
Jose Rivera
Carmen Ramos
Rosangela Rivera
Total Number:

29

Names of personnel receiving PHDs

NAME

Maik Irrazabal

Sandra N. Correa-Torres

Ricardo Infante-Castillo

Michael L. Ramirez

Alvaro Peña-Quevedo

Oliva M. Primera-Pedrozo

Leonardo C. Pacheco-Londoño

Total Number:**7****Names of other research staff**NAMEPERCENT SUPPORTED

Denisse Negrón

1.00 No

Luis de la Torre

1.00 No

Marjorie Pratts

1.00 No

FTE Equivalent:**3.00****Total Number:****3****Sub Contractors (DD882)****Inventions (DD882)****Scientific Progress**

DoD-UPRM-MURI grant: "Establishment of a Center for Development of Chemical Sensors for Explosives at University of Puerto Rico – Mayaguez" (Proposal # 43567CHMUR; Agreement #: DAAD190210257) operated between 2002 and 2010. The project established a multidisciplinary research center for detection of landmine explosives, focusing on spectroscopic signatures of landmines explosives and transport in soil, contributing to real time chemical sensing of landmines. Goals included:

- * Measurement of spectroscopic signatures of landmine explosives in soil;
- * Measurement of effect of environmental variables on explosives;
- * Studies of soil-explosives interactions: Raman and IR spectroscopies
- * Model transport behavior of explosives in soils under different environmental conditions.

The major accomplishments during 8 years of the DoD-MURI-UPRM CCSD:

1. COMPONENT I:

TRANSPORT PHENOMENA OF EXPLOSIVE COMPONENTS IN SOIL: PHYSICAL MODELING

- ☐ Dissemination of results: results were presented at several scientific meetings. Several papers were published in peer review journals.
- ☐ Fate and transport experiments were conducted for 2-4 DNT and 2,4,6-TNT. Experimental work resulted in large amount of data used to advance scientific knowledge on the effect of environmental factors on the fate and transport of ERCs. The data also served to validate models used in the prediction of ERCs fate and transport.
- ☐ Technical accomplishments advance knowledge on fate and transport processes controlling the movement of TNT and DNT in water and vapor phases when subjected to variable environmental conditions, including: variable infiltration and evaporation events, light radiation, temperature, water flux, water content, vegetation, and boundary conditions.
- ☐ Diffusion, dissolution, sorption, and advective/dispersive properties were assessed for 2,4-DNT and 2,4,6-TNT under different environmental conditions.
- ☐ All physical models were built and instrumented. All lab-scale models and a field lysimeter are operational.
- ☐ Samplers and sampling methodology were developed for selectively sampling ERCs in the gas and liquid phase.
- ☐ Methods for analysis of large number of low-volume samples were developed.
- ☐ Fate and transport experiments were conducted for 2-4 DNT and 2,4,6-TNT.
- ☐ Two-Dimensional transport of TNT experiments were conducted under infiltration and evaporation conditions at different environmental conditions.
- ☐ TNT and DNT transport experiments were conducted in 3D laboratory-scale soil tanks under cyclic radiation and precipitation conditions.
- ☐ Effects of vegetation of fate, transport, and detection were studied.
- ☐ Diffusion, dissolution, sorption, and advective/dispersive properties were assessed for 2,4-DNT and 2,4,6-TNT under different environmental conditions.
- ☐ Field measurements and transport experiments were conducted.
- ☐ Twenty-two students from environmental, geotechnical, mechanical, chemical engineering, and soils were trained for the reported period on ERC fate and transport concepts in a multidisciplinary environment.

2. COMPONENT II:

NUMERICAL MODELING OF TRANSPORT PHENOMENA OF LANDMINE EXPLOSIVES AND DEGRADATION PRODUCTS IN SOIL

- ☐ Dissemination of results was significant, including 7 publication, 6 oral presentations, and 8 posters at scientific meetings and workshops.
- ☐ The numerical code was completely validated.
- ☐ 1d, 2d, 3d situations has been studied and published or presented in scientific meetings.
- ☐ The effect of environmental parameters on the chemical signature of TNT was approached both numerically and experimentally.
- ☐ The adsorption of TNT and degradation products on organic matter (humic and fulvic acids) was numerically approached.

3. COMPONENT III:

THEORETICAL UNDERSTANDING OF LANDMINE EXPLOSIVES: PROPERTIES AND BEHAVIOR IN SOIL

- ☐ Several papers and presentations were delivered in the SPIE Defense and Security Meetings and in peer reviewed journals.
- ☐ Computational models have been used to describe the spectroscopic signature of RDX, TNT, and 2,4-DNT.
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- ☐ Ten students from Chemistry, Environmental and chemical engineering and chemistry were trained on ERC fate, transport and detection concepts in a multidisciplinary environment.

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SOIL-EXPLOSIVES INTERACTIONS PROPERTIES UNDER AMBIENT CONDITIONS USING FLUORESCENCE AND PHOTOCHEMISTRY

- ☐ Tested successfully NIR for detection of explosives on surfaces.
- ☐ Established the optical properties of sunlight exposed TNT.
- ☐ Published 1 paper and submitted two additional manuscripts to peer review journals;
- ☐ Submitted two abstracts for SPIE Defense and Security Symposium;
- ☐ Established the N 1s binding energies in RDX

5. Component V:

SPECTROSCOPIC SIGNATURES OF LANDMINE EXPLOSIVES

- ☐ Graduated 25 MS students and 6 Ph.D. students.
- ☐ Studied polymorphism effects on ERCs signatures.
- ☐ Studied nucleation and crystallization properties of TNT and RDX.
- ☐ Began working on Fiber Optic Couple FTIR detection of explosives on surfaces.
- ☐ Used Chemometrics of spectroscopic measurements.
- ☐ Worked on nanotechnology based detection of explosives and other threat chemicals.
- ☐ Designed and developed a Raman based telescope system used in detection of explosives components of Improvised Explosive devices.
- ☐ Started taking data with the home built Raman based telescope system used in detection of explosives.
- ☐ Acquired two Deep Ultra Violet (DUV) Raman Spectrometers: one operating at fixed wavelengths: 244-248 nm and 257 nm. The second system is a triple monochromator Raman Spectrometer, which allowed for variable excitation laser in the DUV, Near UV (NUV) and VIS regions of the spectrum.
- ☐ Presented a component in Department of Homeland Security Center of Excellence for Explosives Detection, Mitigation and Response. The UPRM DoD-MURI Center for Chemical Sensors Development will be part of Northeastern University and University of Rhode Island jointly co-leads DHS-COE.
- ☐ Computational models of spectroscopic signatures: RDX, TNT, DNT, TATP.
- ☐ TNT adsorption properties measured.
- ☐ Calculations of soil-TNT interactions.
- ☐ Published second paper on vibrational spectroscopy standoff detection of explosives; published chapter on state of art of vibrational spectroscopy standoff detection of explosives.
- ☐ Started experiments on remote IR detection of explosives/homemade explosives

Technology Transfer

REPORT DOCUMENTATION PAGE			Form Approved OMB NO. 0704-0188
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FINAL PROGRESS REPORT – 4 FEBRUARY 2011

**ESTABLISHMENT OF A
CENTER FOR DEVELOPMENT OF CHEMICAL SENSORS FOR EXPLOSIVES
AT
UNIVERSITY OF PUERTO RICO – MAYAGÜEZ**

**MURI-ARO-NVL-DOD
Project P43567-CH-MUR-02148-1**

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II.	PROJECT SUMMARY AND PROJECT BUDGET EXPENDITURES AND FORECAST	37
A.	YEARLY EXPENDITURES COMPARISON	37

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- * Measurement of spectroscopic signatures of landmine explosives in soil;
- * Measurement of effect of environmental variables on explosives;
- * Studies of soil-explosives interactions: Raman and IR spectroscopies
- * Model transport behavior of explosives in soils under different environmental conditions.

The major accomplishments during 8 years of the DoD-MURI-UPRM CCSD:

1. COMPONENT I:**TRANSPORT PHENOMENA OF EXPLOSIVE COMPONENTS IN SOIL: PHYSICAL MODELING**

- Dissemination of results: results were presented at several scientific meetings. Several papers were published in peer review journals.
- Fate and transport experiments were conducted for 2-4 DNT and 2,4,6-TNT. Experimental work resulted in large amount of data used to advance scientific knowledge on the effect of environmental factors on the fate and transport of ERCs. The data also served to validate models used in the prediction of ERCs fate and transport.
- Technical accomplishments advance knowledge on fate and transport processes controlling the movement of TNT and DNT in water and vapor phases when subjected to variable environmental conditions, including: variable infiltration and evaporation events, light radiation, temperature, water flux, water content, vegetation, and boundary conditions.
- Diffusion, dissolution, sorption, and advective/dispersive properties were assessed for 2,4-DNT and 2,4,6-TNT under different environmental conditions.
- All physical models were built and instrumented. All lab-scale models and a field lysimeter are operational.
- Samplers and sampling methodology were developed for selectively sampling ERCs in the gas and liquid phase.
- Methods for analysis of large number of low-volume samples were developed.
- Fate and transport experiments were conducted for 2-4 DNT and 2,4,6-TNT.
- Two-Dimensional transport of TNT experiments were conducted under infiltration and evaporation conditions at different environmental conditions.
- TNT and DNT transport experiments were conducted in 3D laboratory-scale soil tanks under cyclic radiation and precipitation conditions.
- Effects of vegetation of fate, transport, and detection were studied.
- Diffusion, dissolution, sorption, and advective/dispersive properties were assessed for 2,4-DNT and 2,4,6-TNT under different environmental conditions.
- Field measurements and transport experiments were conducted.
- Twenty-two students from environmental, geotechnical, mechanical, chemical engineering, and soils were trained for the reported period on ERC fate and transport concepts in a multidisciplinary environment.

**2. COMPONENT II:
NUMERICAL MODELING OF TRANSPORT PHENOMENA OF LANDMINE EXPLOSIVES
AND DEGRADATION PRODUCTS IN SOIL**

- Dissemination of results was significant, including 7 publication, 6 oral presentations, and 8 posters at scientific meetings and workshops.
- The numerical code was completely validated.
- 1d, 2d, 3d situations has been studied and published or presented in scientific meetings.
- The effect of environmental parameters on the chemical signature of TNT was approached both numerically and experimentally.
- The adsorption of TNT and degradation products on organic matter (humic and fulvic acids) was numerically approached.

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THEORETICAL UNDERSTANDING OF LANDMINE EXPLOSIVES: PROPERTIES AND
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I. REPORT DOCUMENTATION PAGE (SF298) (Continuation Sheet)

1. LIST OF PAPER DURING THE REPORTING PERIOD

A. PUBLICATIONS IN PEER REVIEW JOURNALS: 35

1. Espinosa-Fuentes, E.A., Peña-Quevedo, A.J., Pacheco-Londoño, L.C., Infante-Castillo, R. and Hernández-Rivera, S.P., A Review of Peroxide Based Homemade Explosives: Characterization and Detection, in "Explosive Materials: Classification, Composition and Properties", Janssen, T.J., ed., Chemical Engineering Methods and Technology Series, Nova Science Publishers, Inc. Hauppauge, NY, fourth quarter **2010**, ISBN: 978-1-61761-188-9.
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220. Bibiana Báez, *Detection of Explosives in Soils using SPME with Gas Chromatography and TEEM –Mass Spectrometry*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November **2005**.
221. Edwin de la Cruz, *Surface Enhanced Raman Spectroscopy of 2,4,6-Trinitrotoluene in Anatase Nanocrystal*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November **2005**.
222. Indira Jerez-Rozo, *Raman Scattering of Nitroexplosives on Nanoscaled Substrates: Tungsten Trioxide, Copper (I) Oxide, Molybdenum (VI) Oxide, Tin (IV) Oxide, Cobalt (II, III) Oxide, Cerium (IV) Oxide And Scandium Oxide*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November **2005**.
223. Leonardo C. Pacheco, *Nitroexplosives Classification by Molecular Descriptors*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.
224. Luz M. Ballesteros, *Raman Spectroscopic Signatures of PETN in Soil*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November **2005**.
225. Gloria M. Herrera, *Vibrational Raman Signatures of TNT in Contact with Sand Particles*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.
226. Marcia del R. Balaguera, *SERS(S) of Metal Colloidal Polymeric Film*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November 2005.
227. Michael L. Ramírez, *Thermal Ink Jet Based Sample Transfer Techniques for Explosives Detection*, XXIX American Chemical Society Senior Technical Meeting, Lajas P.R., November **2005**.
228. Hernandez-Rivera, S.P., "Spectroscopic Signature of Landmine Components in Soil and its Equilibrium Vapor: The First Step Towards Real-Time Landmine Sensing", 7th Annual Army Landmine Basic Research Technical Review Meeting, Alexandria, VA, February 24-25, **2004**.
229. Hernández-Rivera, S.P., "Detection of Explosives via Spectroscopic Signatures", Workshop for Improvised Explosive Device (IED) Locating Through Explosives Detection, Night Vision and Electronic Sensors Directorate, Institute for Defense Analysis, Alexandria, VA, July 1, **2004**.

2. DEMOGRAPHIC DATA FOR THE REPORTING PERIOD: DISSEMINATION

- a. Number of manuscripts – **146**
- b. Number of Peer Reviewed Papers – **27**
- c. Number of Non-Peer Reviewed Papers – **119**
- d. Number of Presented but not Published Papers – **229**

3. DEMOGRAPHIC DATA FOR THE LIFE OF THIS AGREEMENT:

- a. Number of Scientists Supported by the Project – **8**
- b. Number of Inventions as a result of the Project – **2**
- c. Number of PhD awarded as a result of the Project – **7**
- d. Number of BS awarded as a result of the Project – **30**
- e. Number of Patents Submitted as a result of the Project – **2**
- f. Number of Patents Awarded as a result of the Project – **0**
- g. Number of Graduate Students Supported by the Project – **70**
- h. Number of FTE Graduate Students Supported by the Project – **30**
- i. Number of Post Doctorate Students supported by the Project – **2**

- j. Number of FTE Post Doctorate Students supported by the Project – **0**
- k. Number of Faculty supported by the Project – **8**
- l. Number of Other Staff supported by the Project – **4**
- m. Number of Undergraduate Students supported by the Project – **61**
- n. Number of MS awarded as a result of the Project – **25**

1. STUDENT METRICS FOR GRADUATING UNDERGRADUATES FUNDED BY THIS AGREEMENT

- a. Number of undergraduates funded by your agreement during this reporting period-**61**
- b. Number of undergraduates funded by your agreement, who graduated during this reporting period-**61**
- c. Number of undergraduates funded by your agreement, who graduated during this reporting period with a degree in science, mathematics, engineering, or technology field-**58**
- d. Number of undergraduates funded by your agreement, who graduated during this reporting period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology field- **45**
- e. Number of undergraduates funded by your agreement, who graduated during this reporting period and intend to work for the Department of Defense- **5**
- f. Number of undergraduates graduating during this period, who achieve at least a 3.5 GPA based on a scale with a maximum of a 4.0 GPA- **27**
- g. Number of undergraduates working on your agreement, who graduated during this period and were funded by a DoD Center of Excellence for Education, Research or Engineering - **0**
- h. Number of undergraduates funded by your agreement, who graduated during this period and will receive a scholarship or fellowship for further studies in a science, mathematics, engineering, or technology field-**5**

5. REPORT OF INVENTIONS" NONE

2. SCIENTIFIC PROGRESS AND ACCOMPLISHMENTS:
Included as part of Executive Summary

7. TECHNOLOGY TRANSFER: NONE

II. PROJECT SUMMARY AND PROJECT BUDGET EXPENDITURES AND FORECAST

This project involved a team of scientist, engineers and students at all levels from undergraduate students to post doctoral trainees. It consists of a truly multidisciplinary effort directed to tackle the problem of laying the grounds to design and built real-time, point detection sensors to detect explosive chemicals present in landmines. The project infrastructure consists of four fully interacting components. These groups often merge in joint purposes to achieve common goals and achieving the maximum possible interaction between students, investigators and support personnel. Expertise in areas of chemical detection combine with theoretical computations, numerical and physical environmental modeling to provide a complete research package working together to achieve the program goal: to provide background information on chemical signatures of landmine explosives so that real-time, point detected sensors for detection of landmine explosives may be designed and built at commercial scale.

The total granted money for 2002-10: \$5,444,700

